

# Accuracy Based Generation of Thermodynamic Properties for Light Water in RELAP5-3D

## 2010 RELAP5 International Users Group Meeting

Cliff B. Davis

September 2010

The INL is a  
U.S. Department of Energy  
National Laboratory  
operated by  
Battelle Energy Alliance



This is a preprint of a paper intended for publication in a journal or proceedings. Since changes may be made before publication, this preprint should not be cited or reproduced without permission of the author. This document was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor any agency thereof, or any of their employees, makes any warranty, expressed or implied, or assumes any legal liability or responsibility for any third party's use, or the results of such use, of any information, apparatus, product or process disclosed in this report, or represents that its use by such third party would not infringe privately owned rights. The views expressed in this paper are not necessarily those of the United States Government or the sponsoring agency.

## **Accuracy Based Generation of Thermodynamic Properties for Light Water in RELAP5-3D**

Cliff B. Davis  
Idaho National Laboratory  
2010 RELAP5 International User's Group Meeting  
West Yellowstone, MT  
September 20-23, 2010

### **Abstract**

RELAP5-3D interpolates to obtain thermodynamic properties for use in its internal calculations. The accuracy of the interpolation was determined for the original steam tables currently used by the code. The results of this accuracy evaluation showed that the original steam tables are generally detailed enough to allow reasonably accurate interpolations in most areas needed for analyses of nuclear reactors cooled by light water. However, there were some areas in which the original steam tables were judged to not provide acceptably accurate results. Revised steam tables were created that used a finer thermodynamic mesh between 4 and 21 MPa and 530 and 640 K. The accuracies of the original and revised steam tables were compared throughout the thermodynamic grid. The revised steam tables solved most of the problems observed with the original steam tables.

### **Summary**

RELAP5-3D interpolates to obtain thermodynamic properties for use in its internal calculations. The accuracy of the interpolation was determined for the original steam tables currently used by the code for six basic and five derived thermodynamic properties throughout the entire thermodynamic grid allowed for light water. The results of this accuracy evaluation showed that the original thermodynamic grid is sufficiently detailed to provide acceptably accurate interpolations for most of the regions required for analyses of most nuclear reactors cooled by light water. However, the evaluation also indicated that there were areas where the original thermodynamic grid was not adequate, even in the "normal" liquid and vapor regions needed for analysis of commercial light water reactors. The largest errors were located in the vapor near the saturation line, particularly just above the normal operating pressure of 15 MPa for a pressurized water reactor. The original steam tables were also judged to be inadequate for vapor temperatures between 800 and 1073.15 K.

Revised steam tables were created that used a finer temperature mesh between 530 and 640 K and between 800 and 1073.15 K and a generally finer pressure mesh between 4.0 and 21.5 MPa. The number of temperature points in the thermodynamic grid was increased from 113 to 144 and the number of pressure points was increased from 98 to 126. The revised steam tables significantly reduced the relatively large errors that were sometimes observed in normal liquid and vapor regions. However, the more detailed steam tables did not provide a consistent reduction in mass error for the installation problems. The conclusion from these calculations is that the more detailed steam tables will provide significantly improved results for a few cases, but will probably not have a large impact on most problems. The revisions to the steam tables do not significantly affect the CPU time required to run a problem.

## 1.0 Introduction

RELAP5-3D currently simulates 26 different working fluids, including light and heavy water, several gases, liquid metals, molten salts, and other miscellaneous fluids. Each working fluid contains a full set of thermodynamic and transport properties as a function of pressure and temperature for the saturation line, subcooled liquid, superheated gas, and supercritical fluid. The thermodynamic properties are obtained from an equation of state, while the transport properties are obtained from correlations. The equation of state is used to generate “exact” fluid properties at developer-specified pressures and temperatures that define the thermodynamic grid allowed by the code. To achieve fast running speed, RELAP5-3D obtains the fluid properties for its internal calculations by interpolating between the “exact” fluid properties obtained from the equation of state to obtain approximate thermodynamic properties at any state point. The accuracy of the properties used by RELAP5-3D depends on the number of pressure and temperature points contained in the developer-specified thermodynamic grid as well as the interpolation algorithms used by the code.

The ‘fluids’ directory currently contains ‘.i’ files that the code developers use to specify the pressure and temperature grid points for each fluid. The ‘fluids’ directory also contains ‘.f’ files that use an equation of state to determine the exact solutions at the grid points contained in the ‘.i’ files. The ‘.f’ and ‘.i’ files are used to generate the ‘tpf’ property files used by the code during its interpolations.

The ‘tpf’ files have been validated based on comparisons between properties calculated with the RELAP5-3D and other sources of data. For many of the older fluids, such as light water, the results of these validation calculations are not documented. The validations that are documented did not systematically test every location within the entire thermodynamic grid. Furthermore, the results of the documented validations are affected by any subsequent changes made to the ‘.i’ files. Historically, the ‘.i’ files have been created based on engineering judgment. The ‘.i’ files have generally increased in size over the years to overcome thermodynamic property errors or mass error problems.

A new, more rigorous approach, referred to as accuracy based property generation, was taken to revise the ‘.i’ file for the light water fluid, h2o. The basic approach was to specify the level of accuracy desired for the thermodynamic properties and let the generating program determine the pressure/temperature mesh required to obtain that level of accuracy. The accuracy based approach was applied only to the h2o fluid, which is based on the 1967 ASME steam tables (Meyer et al., 1967). The process can be extended to the other fluids on an as-needed basis. In particular, it will be relatively easy to use the state points developed for the h2o fluid for the other light water fluids, including h2on (Haar et al., 1984) and h2o95 (Harvey et al, 2000).

The process of accuracy based property generation required several steps, which are described below.

First, the thermodynamic grid for the h2o fluid was divided into fourteen distinct regions, which will be defined in more detail later. An acceptable level of accuracy was then determined based on an evaluation of the accuracy of the current thermodynamic grid. Different levels of accuracy were allowed in different thermodynamic regions because some regions were judged to be more important than others for the analysis of nuclear reactors cooled by light water. For example, the normal operating regions were judged to be more important than those regions near the critical point.

The second step was to modify the generating program, which determines the thermodynamic state at each point defined by the pressure and temperature grid contained in the stgh2o.i file. The generating program was modified to calculate all the thermodynamic properties at the midpoint of each box defined by the thermodynamic grid. Third, the subroutine that RELAP5-3D uses to interpolate between the grid points was modified so that it could be called to calculate the values at the midpoint of each box in the thermodynamic grid. The results of the exact solution from the equation of state and the interpolation were then compared at the midpoint of each box to provide a quantitative measure of the accuracy in each box in the thermodynamic grid. Since the interpolated value equals the exact solution at each corner point, the largest error was expected to occur at the midpoint of the box since it was the farthest point away from all corners. Although not discussed in this paper, an evaluation showed that the error at the midpoint is not necessarily the largest error in the box, but it is representative of the maximum error and therefore the error at the midpoint can be reasonably used to measure the error in a box. Error statistics were generated for each of the six basic thermodynamic variables used by RELAP5-3D as well as five other variables that are derived from the basic variables.

The next step in the process was to compare the maximum errors in each pressure column and temperature row of the thermodynamic grid with the acceptable error for the most important thermodynamic regions. If the maximum errors were greater than the acceptable error, more pressure and/or temperature points were placed in the stgh2o.i file, which resulted in a smaller box and reduced errors. This process was continued until a converged solution was obtained in which acceptable accuracy was obtained for all the regions judged to be important.

Finally, the results of RELAP5-3D test problems with the original and revised tpfh2o files were quantitatively compared. The test problems included the installation problems, as well as new cases that were developed to investigate the accuracy of the original and revised tpfh2o files in certain limiting and/or representative boxes. These quantitative comparisons concentrated on the mass error and CPU time.

The evaluation of the accuracy of the original and revised steam tables was performed using the steam tables from RELAP5-3D Version 2.9.3t, which was the most recent code version available when the evaluation started. The RELAP5-3D calculations described in this report were performed with RELAP5-3D Version 2.9.4t, which was the most recent code version available when the calculations were performed. The steam tables used in the two code versions are identical.

The basic and derived thermodynamic properties used in this evaluation are described in Section 2 of this report. The thermodynamic grid contained in the stgh2o.i file was divided into 14 regions as described in Section 3. Section 4 describes the modifications to the generating program that were made to perform this evaluation. Section 5 presents results from the evaluations of accuracy of the original and revised steam tables. Conclusions and references are provided in Sections 6 and 7, respectively.

## **2. Thermodynamic Properties**

RELAP5-3D accesses six basic thermodynamic properties of light water through tables that are located in an auxiliary, binary file called tpfh2o. The basic thermodynamic properties include specific volume,  $v$ , specific internal energy,  $U$ , the isobaric coefficient of thermal expansion,  $\beta$ , the isothermal coefficient of compressibility,  $\kappa$ , the specific heat capacity at constant pressure,  $C_p$ , and the specific entropy,  $S$ .

The code also utilizes five derived thermodynamic properties that depend on the basic thermodynamic properties. These derived thermodynamic properties include four derivatives that are used in the numerical scheme and the single-phase sound speed and are described in Section 3.2.2 of Volume 1 of the code manual (the RELAP5-3D Code Development Team, 2009). These derived variables are  $\left(\frac{\partial \rho}{\partial U}\right)_P$ ,  $\left(\frac{\partial T}{\partial U}\right)_P$ ,  $\left(\frac{\partial \rho}{\partial P}\right)_U$ ,  $\left(\frac{\partial T}{\partial P}\right)_U$ , and  $a$ , where  $\rho$  is the density,  $P$  is the pressure,  $T$  is the temperature, and  $a$  is the single-phase sound speed.

The accuracy of the code's interpolation for each of the six basic and five derived thermodynamic properties is discussed in Section 5.

### 3.0 Region Definitions

The 1967 ASME steam tables allow the pressure and temperature to vary from the triple point to 100 MPa and 1073.15 K. RELAP5-3D allows temperatures to be entered up to a maximum value of 5000 K, but thermodynamic properties for values above 1073.15 K are calculated using ideal gas assumptions.

For convenience, the thermodynamic pressure and temperature grid was divided into 14 regions in this analysis. Region definitions are illustrated in Figures 1 and 2, where the figures concentrate on the high-pressure and low-pressure ranges, respectively. In both figures, the saturation line is the curved line that runs between the triple ( $P = 6.112\text{E-}04$  MPa and  $T = 273.16$  K) and critical ( $P = 22.12$  MPa and  $647.3$  K) points. Regions 1 and 2 are of the most interest for analyses of light water cooled reactors. The pressure limits for Regions 1 and 2 are 0.1 to 17.52 MPa, which roughly covers the range from atmospheric pressure to the opening setpoint of the safety relief valves on the pressurizer in a pressurized water reactor (PWR). The normal temperature range extends from 294.3 to 627.9 K, which covers the range from room temperature to the saturation temperature corresponding to the pressure setpoint of the safety relief valves. Region 1 is above the saturation line in Figures 1 and 2 and contains liquid. Region 2 is below the saturation line and contains vapor. Region 3 represents high-pressure liquid. The upper range of 27 MPa in Region 3 roughly corresponds to the opening pressure setpoint of the safety relief valves in proposed reactors cooled by supercritical water (MacDonald et al., 2005). Pressures higher than 27 MPa are not considered to be of interest in the current analysis. Region 4 contains high temperature vapor, with the minimum and maximum values ranging between 627.9 and 1073.15 K, where the upper value corresponds to the limit of the ASME steam tables. Although the maximum value does not reach the 2200°F value specified by Appendix K (Nuclear Regulatory Commission, 2010), it is high enough for practical applications.

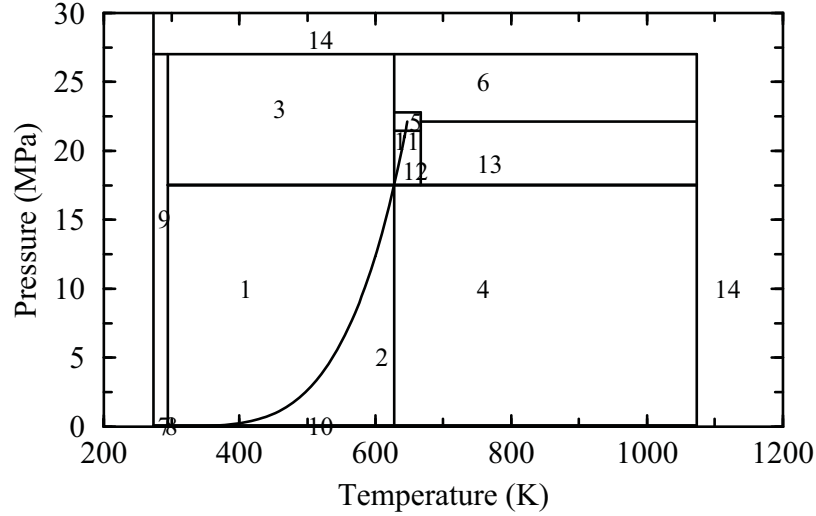


Figure 1. Definition of regions (high pressure).

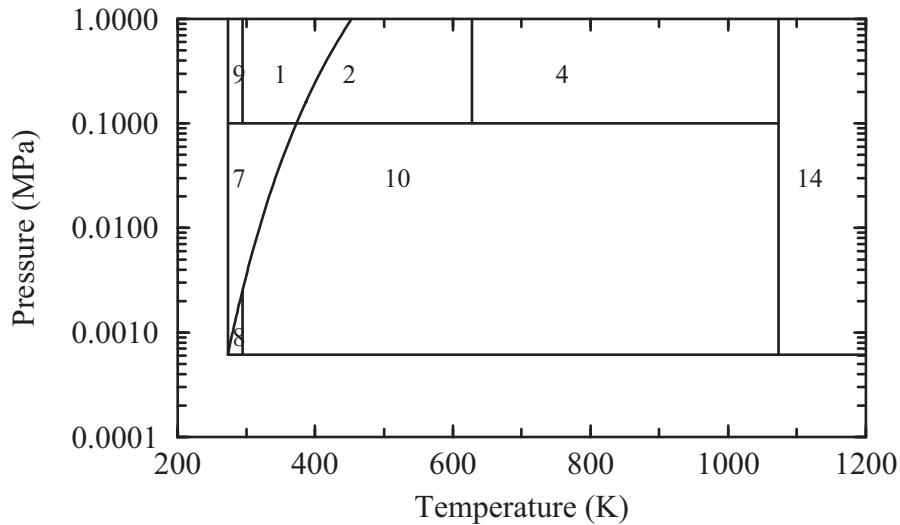


Figure 2. Definition of regions (low pressure).

Region 5 is a small region located around the critical point. The temperature limits for this region vary between 0.97 and 1.03 times the critical value. The pressure limits for this region vary between the saturated value corresponding to 0.97 times the critical temperature to 1.03 times the critical pressure. Region 6 contains supercritical fluid and has maximum values of 27 MPa and 1073.15 K. Regions 7 and 8 contain low-pressure, low-temperature liquid and vapor respectively and are primarily of interest in simulating condensers. Region 9 contains low-temperature liquid, while Region 10 contains low-pressure vapor. Regions 11 and 12 are near the saturation line and the critical point, while Region 13 contains high-pressure, high-temperature vapor. Region 14 contains the remainder of the thermodynamic grid.

Regions 1 and 2 are considered to be the most important regions for the analysis of reactors cooled by light water. Therefore, the thermodynamic properties in Regions 1 and 2 are required

to have relatively high levels of accuracy. Regions 3 and 4 are also considered to be of practical importance in analyses of reactors cooled by light water. Thus, the thermodynamic grid is adjusted as needed to achieve reasonable levels of accuracy in these regions, but the accuracy requirements are not as high as in Regions 1 and 2. As will be shown later, the thermodynamic properties in Regions 7 through 10 were reasonably accurate with the current stgh2o.i file. Therefore, changes to the thermodynamic grid were not required in these regions. The other regions were considered to be of lesser importance for the analysis of reactors cooled by light water, and no changes to the thermodynamic grid were made in these regions.

#### 4.0 Modification of Generating Program

The tpfh2o file contains five tables. The first two tables contain the temperatures and pressures that form the thermodynamic grid and are copies of the temperatures and pressures that are contained in the stgh2o.i file. The third table contains saturation properties as a function of temperature. The temperature values vary between the triple and critical points. The fourth table contains saturation properties as a function of pressure. The pressures in this table also vary between the triple and critical points. The fifth table contains single-phase thermodynamic properties that correspond to the pressure/temperature grid points.

Figure 3 illustrates a small portion of the thermodynamic grid. The temperatures and pressures input in the stgh2o.i file for this portion of the grid are 365, 370, and 375 K and 0.06, 0.08, and 0.10 MPa, respectively. The saturation properties determined from the input temperatures are placed in the third table. The saturation properties determined from the input pressures are placed in the fourth table. The grid points are defined by the intersection of the vertical temperature lines and the horizontal pressure lines. The generating program determines the thermodynamic properties at each grid point from the ASME subroutines and places them in the fifth table. The properties calculated by the generating program are considered exact in subsequent discussions.

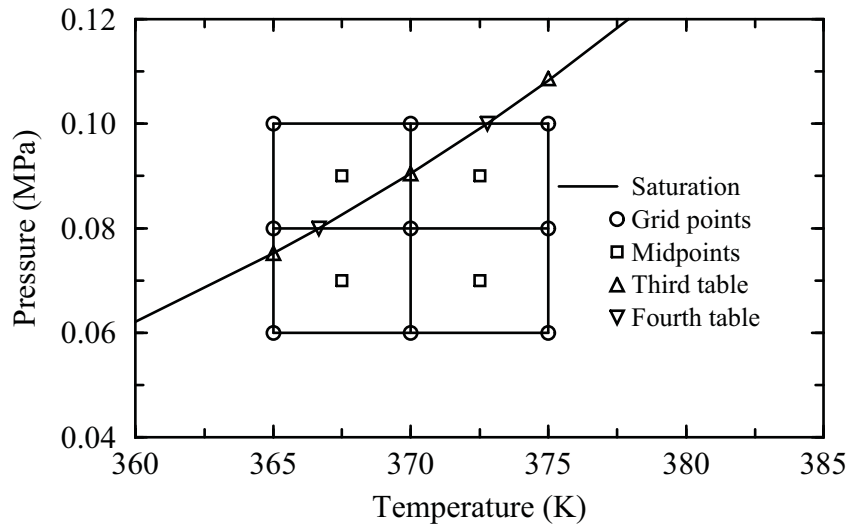


Figure 3. Illustration of the thermodynamic grid.

RELAP5-3D determines fluid properties by interpolating between the exact properties contained in the tpfh2o file. Away from the saturation line, the interpolations are performed using the adjacent four grid points contained in the fifth table of the tpfh2o file. For example, fluid



properties in the lower right box in Figure 3 are interpolated from the exact values at the grid points defined at 370 and 375 K and 0.06 and 0.08 MPa. For boxes near the saturation line, the interpolations are performed between grid points contained in the fifth table and saturated properties obtained from either the third or fourth tables. The accuracy of the interpolated properties depends on accuracy of the interpolating algorithms compared to the actual generating functions and the size of the box.

A driver program was written to perform all the calculations described in this report. The driver program is based on the generating program that is used to create the `tpfh2o` file. The generating program was modified to calculate and store the thermodynamic properties at the midpoint of each box. The generating program was also modified to obtain midpoint properties with the same interpolations used by RELAP5-3D. These interpolations were based on Subroutine `sth2x3`, which RELAP5-3D uses to determine thermodynamic properties when the independent variables are pressure and temperature. The generating program was also modified to compare the exact and interpolated thermodynamic values at box midpoints and to generate statistics concerning the average, root mean square, and maximum error for each of the fourteen regions in the thermodynamic grid.

The driver program also adjusts the pressure/temperature grid to obtain a desired level of accuracy for a given thermodynamic property. This process required several steps. First, the normalized error,  $E$ , at the midpoint of each box in the thermodynamic grid was calculated as

$$E = \left| \frac{X_I - X_G}{X_G} \right|, \quad (1)$$

where  $X_I$  and  $X_G$  were the values of the property from the interpolator and generator, respectively. The ratio,  $R$ , of the normalized error to a desired error,  $\varepsilon$ , was then calculated as

$$R = \frac{E}{\varepsilon}. \quad (2)$$

If  $R$  was less than 2.0, the existing box was judged to be adequate and no changes in the box size were made for the next iteration. If  $R$  was greater than 2.0, the area of the box was reduced by a factor of 2.0 for the next iteration. Since the worst box (based on  $R$ ) in each pressure row and temperature column must meet the accuracy criterion, the worst box in a pressure row determines the new differential pressure ( $dP$ ) for the entire row. Similarly, the worst box in a temperature column determines the new temperature difference ( $dT$ ) for the entire column. The process is illustrated graphically in Figure 4.



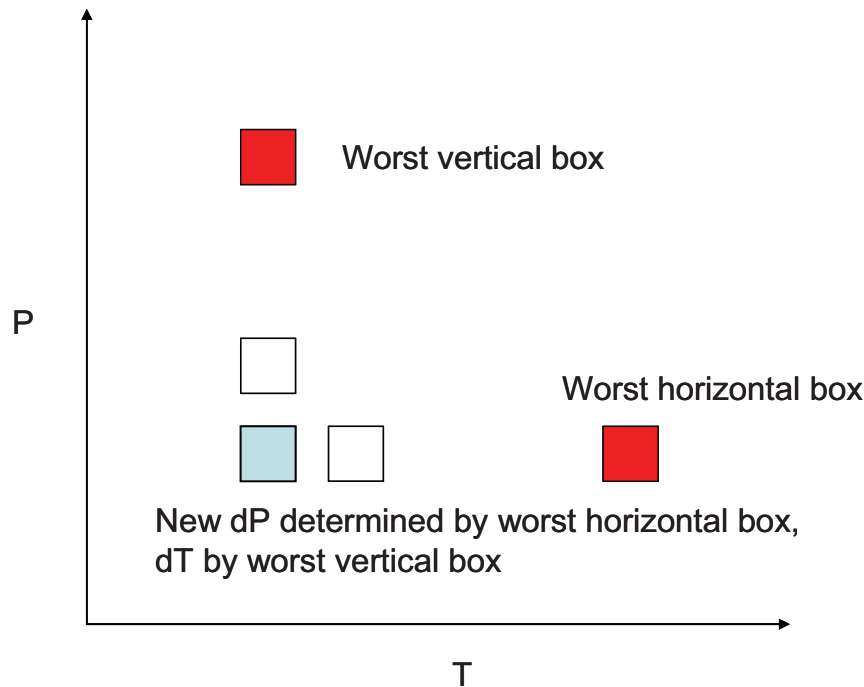


Figure 4. Illustration of approach for the determination of new box size.

Changes to the thermodynamic grid were made only in Regions 1 and 2 and in parts of Regions 3, 4, and 10 through 12. The changes in Regions 1 and 2 were based on the process illustrated in Figure 4. Reducing the box area by a factor of 2.0 was accomplished by reducing the pressure and temperature intervals each by a factor of  $\sqrt{2.0}$ . Changes to the thermodynamic grid in Regions 3 and 4 were made in such a manner as to avoid changes near the critical point. Therefore, the changes were made to the lower part of Region 3 and the right part of Region 4 shown in Figure 1. Specifically, the pressure intervals in the lower part of Region 3 were adjusted using the worst R ratio for pressures less than 21.5 MPa. Reductions in box area were accomplished by reducing the pressure interval by a factor of 2.0. The temperature intervals in the right part of Regions 4 and 10 were adjusted using the worst R ratio for temperatures greater than 668 K. Reductions in box area were accomplished by reducing the temperature interval by a factor of 2.0. The temperature intervals in Regions 11 and 12 were allowed to be about 3.0 K for temperatures less than 640 K. Although arbitrary, this temperature interval was smaller than the 5.0 K contained in the original grid, but was larger than the converged temperature interval of 1.0 K for adjacent intervals in Regions 1 and 2. A larger interval was allowed in Regions 11 and 12 because these regions were not judged to be as important for analysis of reactors cooled by light water. Changes to the pressure and temperature grids in the other regions were not made because the accuracy of the existing grid was judged to be adequate or the regions were judged not to be important for the analysis of reactors cooled by light water.

Except for the triple and critical points, each pressure/temperature pair in the thermodynamic grid generally does not lie on the saturation line. If the pressure/temperature pair is “too close” to the saturation line, the generating program will automatically set the thermodynamic properties in the fifth table to those of saturated liquid. If the thermodynamic state of the pressure/temperature pair is actually liquid, the differences between saturated and subcooled properties are small and the consequences of setting the properties to those of saturated liquid are insignificant. However, if the thermodynamic state of the pressure/temperature pair is vapor, setting the vapor properties

to those of saturated liquid can cause the code to fail because the vapor properties in the affected box will be calculated from an interpolation that includes liquid values, which will vary significantly from the correct vapor values away from the critical point. The generating program defines that a pressure/temperature pair is “too close” to the saturation line if the variable *rdiff* is too small, or

$$\text{rdiff} = \left| \frac{T - T_{\text{sat}}}{T} \right| < 0.0001, \quad (3)$$

where  $T_{\text{sat}}$  is the saturation temperature calculated from the pressure. If *rdiff* of a pressure/temperature pair in the revised grid is  $< 0.0002$ , the driver program will adjust either the temperature or the pressure so that *rdiff* = 0.0002. The criterion that the pressure/temperature pair is not too close to the saturation line effectively places a limit on how small the pressure and temperature intervals can be. Specifically, the temperature interval must be greater than 0.13 K and the pressure interval must be greater than 0.004 times the pressure in order to assure that there is sufficient room to move temperature or pressure points to achieve a *rdiff* value of at least 0.0002. The driver program currently sets minimum values of 1 K for the temperature interval and 0.01 times the midpoint pressure for the pressure interval to avoid problems with having points too close to the saturation line.

## 5.0 Results

The results of the evaluation of accuracy in the interpolations at box midpoints for the original and revised *stgh2o.i* files are discussed in Sections 5.1 and 5.2, respectively. Section 5.3 summarizes the effects of the revision to the steam tables on various RELAP5-3D calculations.

### 5.1 Original *stgh2o.i* File

The pressure and temperature points contained in the original *stgh2o.i* file used during this evaluation are shown in Table 1.

Table 1. Pressure and temperature points used in the original steam tables.

113 temperatures as follows:

273.16	277.5	280.	282.5	285.	287.5	290.	292.5	295.	297.5
300.	302.5	305.	307.5	310.	312.5	315.	320.	325.	330.
335.	340.	345.	350.	355.	360.	365.	370.	375.	380.
390.	400.	420.	440.	460.	480.	500.	510.	520.	530.
540.	550.	560.	570.	580.	590.	595.	600.	605.	610.
615.	620.	625.	630.	635.	640.	642.	643.	644.	645.
646.	647.3	648.	648.5	649.	649.5	650.	650.5	651.	651.5
652.	652.5	653.	653.5	654.	654.5	655.	656.	657.	658.
659.	660.	662.	664.	666.	668.	670.	675.	680.	685.
690.	695.	700.	710.	720.	730.	740.	750.	760.	770.
780.	790.	800.	1073.15	1450.	1800.	2200.	2600.	3000.	3500.
4000.	4500.	5000.							

98 pressures as follows:

611.2445	1.e3	1.2e3	1.4e3	1.6e3	1.8e3
2.e3	4.e3	5.e3	6.e3	10.e3	15.e3
20.e3	30.e3	40.e3	50.e3	60.e3	80.e3
100.e3	125.e3	150.e3	160.e3	175.e3	200.e3
250.e3	300.e3	320.e3	350.e3	400.e3	500.e3
600.e3	630.e3	700.e3	800.e3	1000.e3	1200.e3
1250.e3	1400.e3	1500.e3	1600.e3	1800.e3	2000.e3
2500.e3	3000.e3	3200.e3	3500.e3	4000.e3	5000.e3
6000.e3	6300.e3	7000.e3	8000.e3	9000.e3	10000.e3
11500.e3	12500.e3	12600.e3	12700.e3	12800.e3	12900.e3
13000.e3	13100.e3	13200.e3	13300.e3	13400.e3	13500.e3
15000.e3	17000.e3	17500.e3	19000.e3	20000.e3	21000.e3
21500.e3	21780.8e3	22120.e3	22500.e3	23000.e3	23500.e3
24000.e3	24500.e3	25000.e3	25500.e3	26000.e3	26500.e3
27000.e3	27500.e3	28000.e3	29000.e3	30000.e3	32000.e3
40000.e3	42000.e3	50000.e3	56000.e3	60000.e3	75000.e3
80000.e3	100000.e3				

The accuracy of the interpolations used with the original stgh2o.i file is summarized in Figures 5 and 6 for Regions 1 and 2, respectively. Each figure shows the average and maximum normalized error from Equation 1 at the midpoints of all the boxes in Regions 1 and 2 for the six basic thermodynamic properties (Parameters 1 through 6) and four derived properties (Parameters 7 through 10). The normalized value for the fifth derived property,  $\left(\frac{\partial T}{\partial P}\right)_U$ , is not included to prevent divides by zero that occur because the derivative is zero when the generator applies ideal gas assumptions in some portions of the thermodynamic grid.

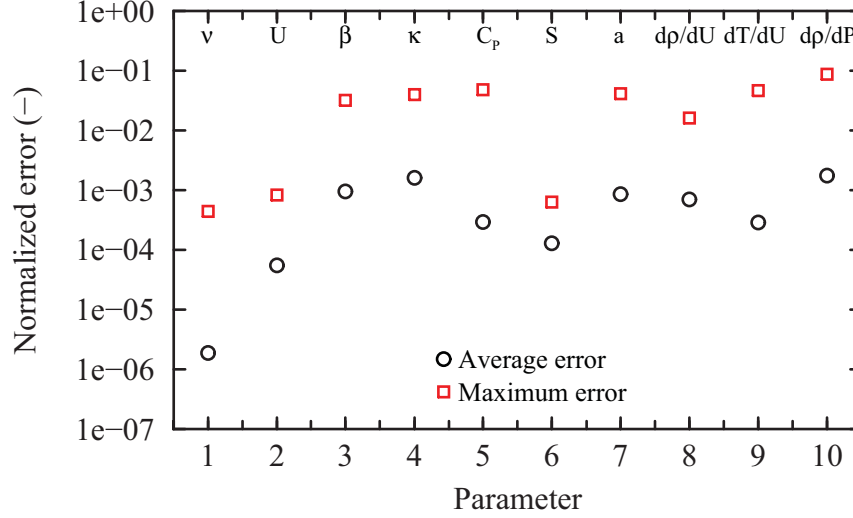


Figure 5. Normalized errors in Region 1 with the original steam tables.

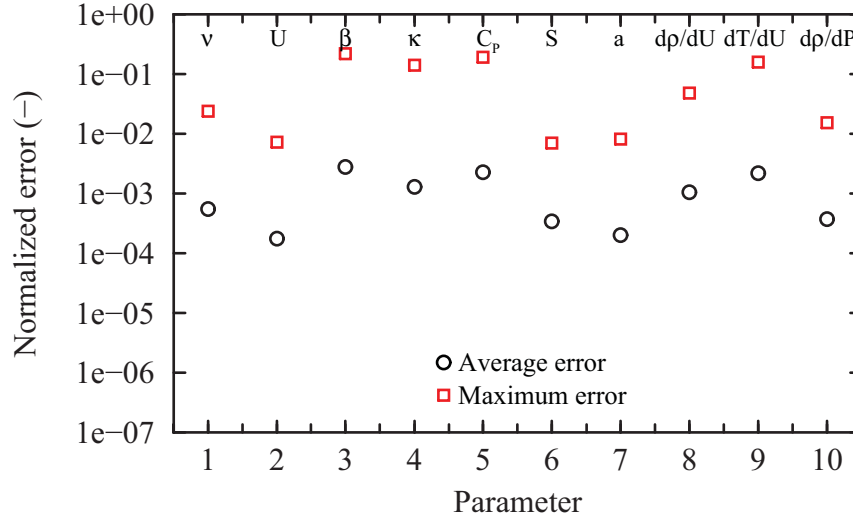


Figure 6. Normalized errors in Region 2 with the original steam tables.

The results shown in Figure 5 correspond to the normal liquid region. The average error is extremely small in the specific volume (Parameter 1), which indicates that the interpolation algorithm used by RELAP5-3D is generally very accurate for subcooled liquid. The average errors are also relatively small for the specific internal energy and specific entropy. The errors in the specific heat capacity and coefficients of thermal expansion and isothermal compressibility are generally at least an order of magnitude higher than the errors in the other basic thermodynamic properties. The errors in the specific heat capacity and coefficients of thermal expansion and isothermal compressibility are expected to be significantly higher than the errors in the other basic properties because they are related to derivatives in the primary properties of specific volume and specific internal energy. The average errors in all the properties based on derivatives (the specific heat capacity, the coefficients of thermal expansion and isothermal compressibility and the derived thermodynamic properties described in Section 2) are similar. This suggests that reducing the error in any of these derivatives would result in a reduction of the

error for all of them. Thus, any of these derivatives could be used as a proxy for the others. The iterations used to determine the revised stgh2o.i file described in Section 5.2 were based on the coefficient of thermal expansion, but it is likely that similar results would have been obtained if any of the derivatives had been used.

Figure 5 also shows that the maximum errors in Region 1 are generally one or two orders of magnitude higher than the average errors. The maximum errors for the derivatives are on the order of a few percent, which are high enough to be of potential concern. This magnitude of error indicates the coarseness of the current thermodynamic grid could negatively affect the overall accuracy of RELAP5-3D calculations in some portions of the normal liquid region. Since the current grid used in the steam tables generally gives acceptable results, a reduction in the maximum errors could result in a significant improvement in overall code accuracy in some regions of the grid. Furthermore, relatively large errors in a few boxes have the potential to significantly affect the overall averages. For example, the combined error from the worst five boxes (out of 1537 in Region 1) is responsible for half of the total error associated in specific volume. The approach taken in this evaluation is to revise the stgh2o.i file to use a finer grid in those regions that produce the maximum errors and leave the original grid as is in those regions where it is judged to give acceptable results.

The results shown in Figure 6 correspond to the normal vapor region. The results are similar to those discussed previously for liquid in that the errors associated with all the derivatives have similar magnitudes, the errors associated with the derivatives are much greater than those associated with the specific volume and specific internal energy, and the maximum errors are one to two orders of magnitude higher than the average errors. However, the average and maximum errors for the vapor are much higher than those shown previously for the liquid. For example, the maximum error in the coefficient of thermal expansion is 0.217 for the vapor versus 0.032 for the liquid. As will be shown later, the relatively large error in the normal vapor region can cause inaccurate code calculations.

Figure 7 shows the normalized error in the specific volume as a function of temperature for five different pressures that vary from 0.1 to 16.0 MPa. The figure shows that the normalized error generally increases with pressure. The largest errors generally occur in vapor near the saturation line. The figure also shows that the original temperature grid uses very large intervals above 800 K. Table 1 shows that the original grid contains no temperature points between 800 and 1073.15 K.

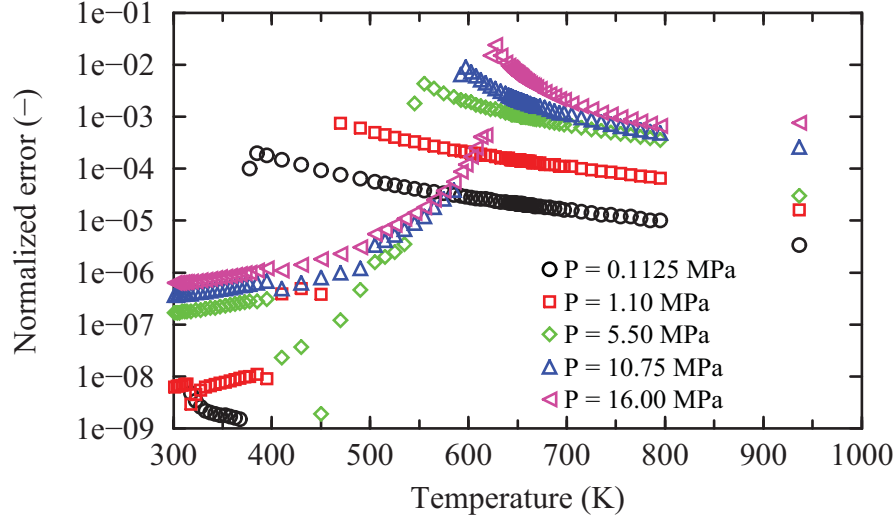


Figure 7. Normalized error in specific volume for the original steam tables.

Figure 8 shows the locations of relatively large normalized errors in specific volume with the original steam tables. A normalized error was considered to be relatively large if it was greater than 0.002, which is nearly four times the average error in Region 2. The figure shows that the relatively large errors were concentrated in the vapor region near the saturation line. The errors were especially large near the critical point and along the pseudo-critical line above the critical point. There was also a region of relatively large errors in Region 6 near 937 K, which corresponds to the midpoint of the large temperature interval between 800 and 1073.15 K.

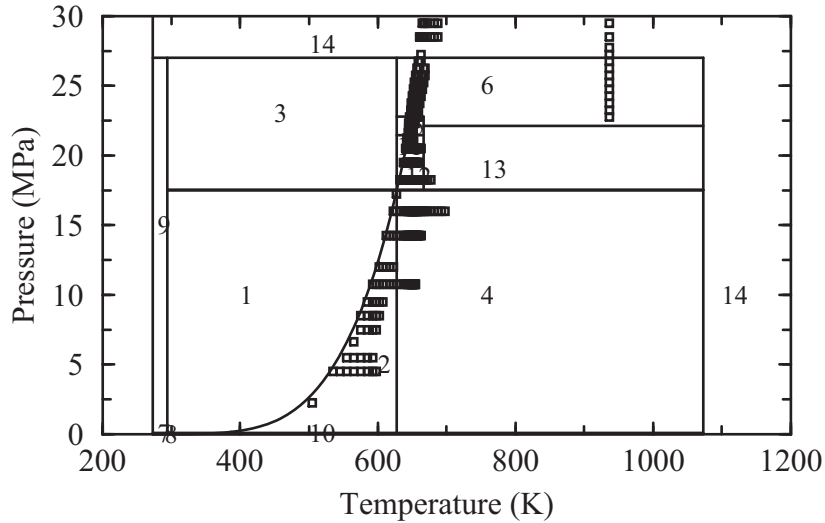


Figure 8. Locations of large normalized errors in specific volume for the original steam tables.

Figure 9 shows the locations of relatively large normalized errors in the coefficient of thermal expansion with the original steam tables. A normalized error was considered to be relatively large if it was greater than 0.01, which is nearly four times the average error in Region 2. The results are similar to those shown in Figure 8 in that points with relatively large errors were clustered in the vapor region near the saturation line. However, there were some liquid points near the saturation line that also had relatively large errors, which was in contrast to the results

shown in Figure 8. The relatively large errors near 937 K also extended down into Regions 13 and 4, where they were limited to Region 6 in Figure 8. Also, there was a cluster of points near 277 K that spanned the entire pressure grid. The liquid density of light water reaches a maximum near 277 K, which causes the coefficient of thermal expansion to become zero. The normalized error becomes large because the denominator in Equation 1 is near zero even though the differences between the interpolator and generator are relatively small. Consequently, the relatively large errors in the coefficient of thermal expansion near 277 K were judged to be insignificant.

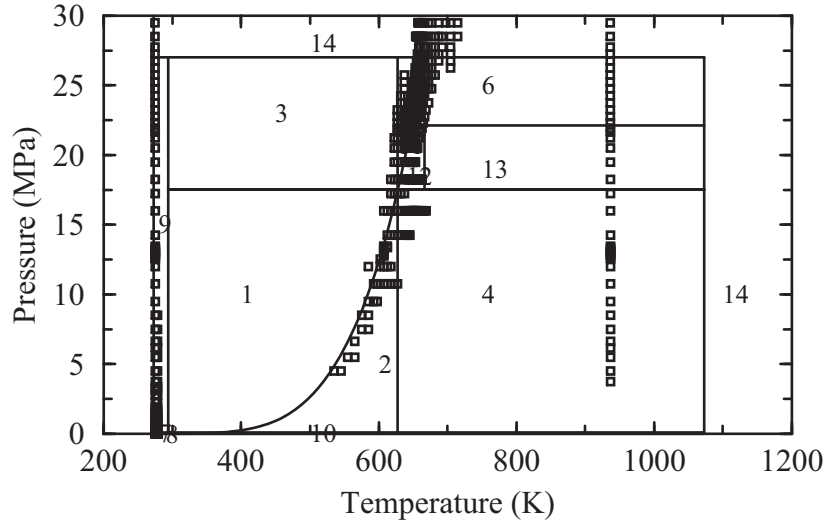


Figure 9. Locations of large normalized errors in the coefficient of thermal expansion for the original steam tables.

## 5.2 Revised stgh2o.i File

A revised stgh2o.i file was created during this evaluation. The revised file was created using the method summarized in Figure 4. The ratio evaluated in Equation 1 was based on the coefficient of thermal expansion. The desired error,  $\epsilon$ , was set to 0.005 for all regions. The original stgh2o.i file was the starting point for the iterations. Convergence was obtained after 10 iterations. The pressure and temperature points contained in the revised stgh2o.i file are shown in Table 2. The revised stgh2o.i file uses a finer temperature mesh between 530 and 640 K and between 800 and 1073.15 K, and is almost identical otherwise to the original temperature mesh. The revised file uses a finer pressure mesh between 4.0 and 21.5 MPa, except between 12.5 and 13.5 MPa, where the pressure intervals were 0.1 MPa in the original mesh and are about 0.25 MPa in the revised mesh. The original and revised files are identical below 4.0 MPa and above 21.5 MPa.



Table 2. Pressure and temperature points used in the revised steam tables.

144 temperatures as follows:

273.16	277.50	280.00	282.50	285.00	287.50	290.00	292.50	295.00
297.50	300.00	302.50	305.00	307.50	310.00	312.50	315.00	320.00
325.00	330.00	335.00	340.00	345.00	350.00	355.00	360.00	365.00
370.00	375.00	380.00	390.00	400.00	420.00	440.00	460.00	480.00
500.00	510.00	520.00	530.00	537.07	544.14	551.21	558.28	565.36
572.43	577.51	582.43	587.43	590.97	594.50	597.00	598.77	600.55
601.79	603.03	604.03	605.28	606.28	607.53	608.78	610.03	611.03
612.03	613.03	614.03	615.03	616.03	617.03	618.03	619.03	620.03
621.03	622.03	623.03	624.03	625.13	626.03	627.03	630.03	633.03
636.03	638.50	640.00	642.01	643.00	644.01	645.00	646.00	647.30
648.00	648.50	649.00	649.50	650.00	650.50	651.00	651.50	652.00
652.50	653.00	653.50	654.00	654.50	655.00	656.00	657.00	658.00
659.00	660.00	662.00	664.00	666.00	668.00	670.00	675.00	680.00
685.00	690.00	695.00	700.00	710.00	720.00	730.00	740.00	750.00
760.00	770.00	780.00	790.00	800.00	834.14	868.29	936.58	1073.15
1450.00	1800.00	2200.00	2600.00	3000.00	3500.00	4000.00	4500.00	5000.00

126 pressures as follows:

611.2445	1.00000E+03	1.20000E+03	1.40000E+03	1.60000E+03	1.80000E+03
2.00000E+03	4.00000E+03	5.00000E+03	6.00000E+03	1.00000E+04	1.50000E+04
2.00000E+04	3.00000E+04	4.00000E+04	5.00000E+04	6.00000E+04	8.00000E+04
1.00000E+05	1.25000E+05	1.50000E+05	1.60000E+05	1.75000E+05	2.00000E+05
2.50000E+05	3.00000E+05	3.20000E+05	3.50000E+05	4.00000E+05	5.00000E+05
6.00000E+05	6.30000E+05	7.00000E+05	8.00000E+05	1.00000E+06	1.20000E+06
1.25000E+06	1.40000E+06	1.50000E+06	1.60000E+06	1.80000E+06	2.00000E+06
2.50000E+06	3.00000E+06	3.20000E+06	3.50000E+06	4.00000E+06	4.70711E+06
5.41421E+06	6.12132E+06	6.42132E+06	6.91630E+06	7.41127E+06	8.11838E+06
8.61838E+06	9.11837E+06	9.61837E+06	1.01184E+07	1.04759E+07	1.08255E+07
1.12005E+07	1.15755E+07	1.19505E+07	1.23256E+07	1.27005E+07	1.29657E+07
1.32402E+07	1.34808E+07	1.37308E+07	1.39960E+07	1.42612E+07	1.45263E+07
1.47138E+07	1.49012E+07	1.50887E+07	1.52763E+07	1.54638E+07	1.56513E+07
1.58388E+07	1.60262E+07	1.62262E+07	1.64013E+07	1.65806E+07	1.67472E+07
1.69155E+07	1.70855E+07	1.72572E+07	1.74963E+07	1.77496E+07	1.80158E+07
1.82680E+07	1.85332E+07	1.87207E+07	1.89088E+07	1.90988E+07	1.94738E+07
1.98488E+07	2.02368E+07	2.06292E+07	2.11228E+07	2.15000E+07	2.17808E+07
2.21200E+07	2.25000E+07	2.30000E+07	2.35000E+07	2.40000E+07	2.45000E+07
2.50000E+07	2.55000E+07	2.60000E+07	2.65000E+07	2.70000E+07	2.75000E+07
2.80000E+07	2.90000E+07	3.00000E+07	3.20000E+07	4.00000E+07	4.20000E+07
5.00000E+07	5.60000E+07	6.00000E+07	7.50000E+07	8.00000E+07	1.00000E+08

The accuracy of the interpolations used with the original and revised stgh2o.i files is summarized in Figures 10 and 11 for Regions 1 and 2, respectively. The open symbols were generated with the original steam tables, while the solid symbols were generated with the revised steam tables. When averaged over ten properties in the normal liquid region, the average errors were reduced by 30% and the maximum errors were reduced by 70% when the detailed steam tables were used. A larger improvement was obtained in the normal vapor region, where the average errors were reduced by 60% and the maximum errors were reduced by more than 80% when the detailed steam tables were used.

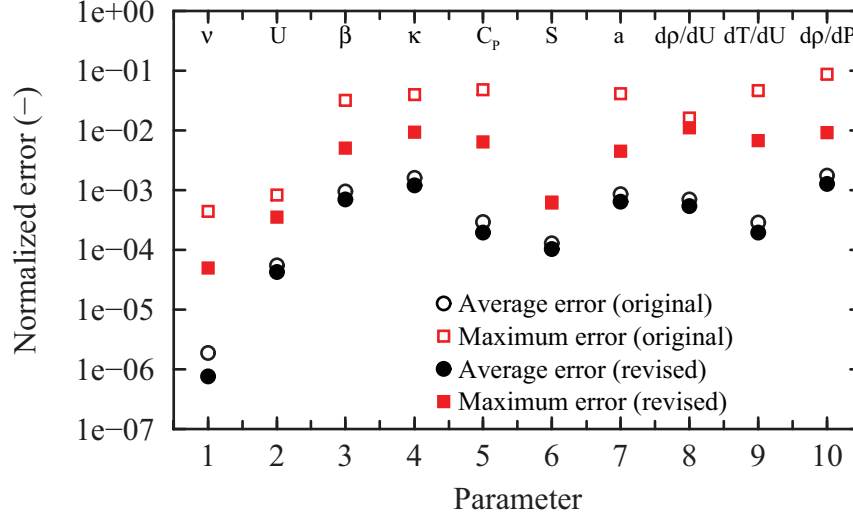


Figure 10. Normalized errors in Region 1 with the original and revised steam tables.

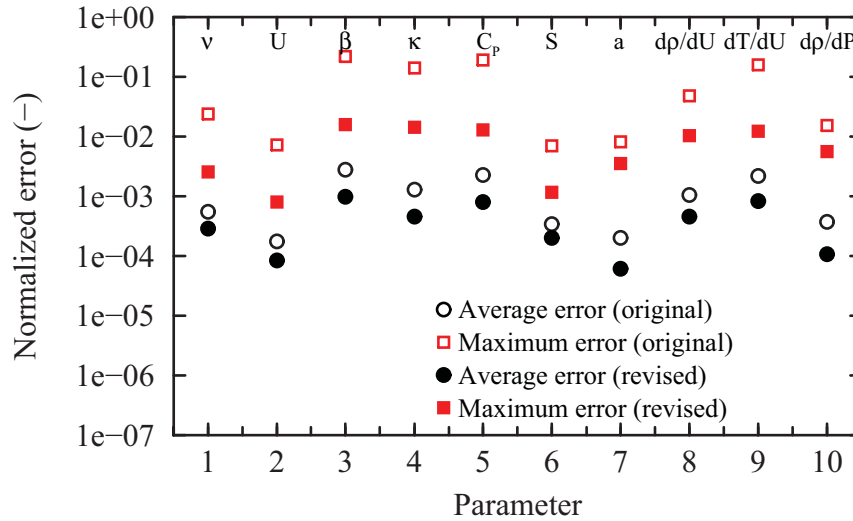


Figure 11. Normalized errors in Region 2 with the original and revised steam tables.

Figure 12 shows the locations of relatively large normalized errors in the coefficient of thermal expansion with the revised steam tables. A normalized error was considered to be relatively large if it was greater than 0.01. The results are significantly improved compared to those obtained with the original steam tables as shown previously in Figure 9. The number of boxes with large errors was reduced from 6 to 0 in Region 1, from 43 to 3 in Region 2, from 14 to 0 in Region 3, and from 66 to 8 in Region 4. Even though the iterations were based on the normalized error in the coefficient of thermal expansion, the number of boxes with large errors did not diminish to zero in Region 2 because these boxes were limited by the minimum interval sizes that were allowed in order to prevent pressure/ temperature pairs from getting too close to the saturation line. Improved results near the critical point would require a reduction in the minimum interval sizes from the current values of 1 K and 1% of the midpoint pressure.

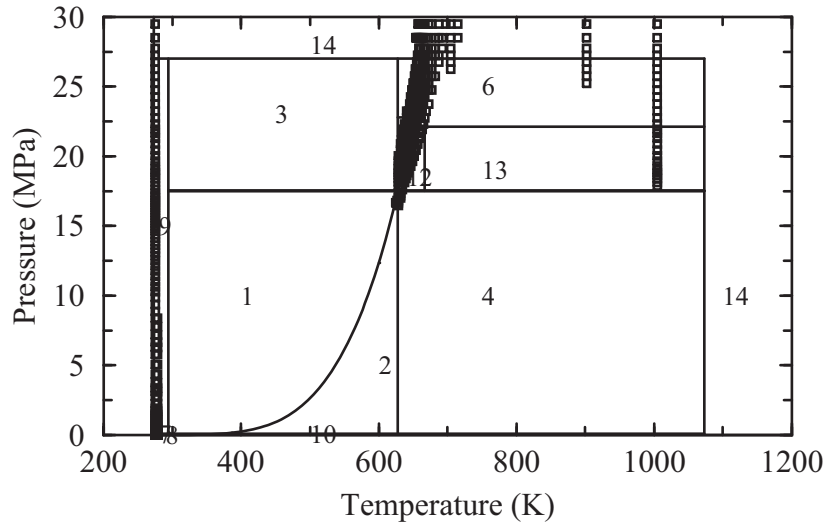


Figure 12. Locations of large normalized errors in the coefficient of thermal expansion in the revised steam tables.

Figure 13 shows the locations of relatively large errors in specific volume with the revised steam tables. A normalized error was considered to be relatively large if it was greater than 0.002. The results are significantly improved compared to those obtained with the original steam tables (see Figure 8), although there were eight boxes that did not meet the desired error criterion in Region 2 for specific volume after convergence with respect to the coefficient of thermal expansion was obtained. This indicates that the error criterion of 0.002 for specific volume is more stringent than the error criterion of 0.01 for the coefficient of thermal expansion for these boxes. The results with the revised steam tables were judged to be adequate because the average error of these eight boxes was 0.00232, which just slightly exceeded error criterion, and Figure 11 shows that use of the revised steam tables significantly reduced the average and maximum errors in specific volume in Region 2.

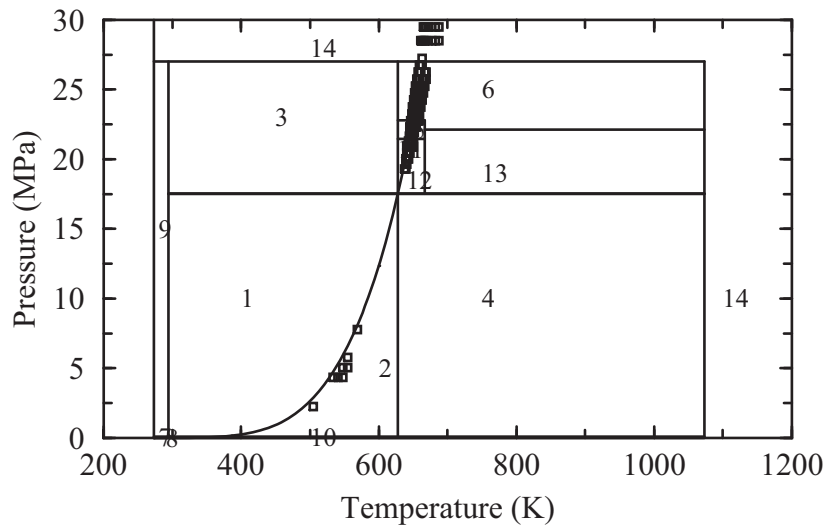


Figure 13. Locations of large normalized errors in the specific volume in the revised steam tables.

### 5.3 Effect of Revisions to Steam Tables on RELAP5-3D Calculations

RELAP5-3D calculations were performed to investigate the code's response during simple fill problems in various boxes in the thermodynamic grid. A two-volume input model was used as illustrated in Figure 14. Component 503 was a single-volume with a geometry that was representative of the pressurizer in a PWR. Component 501 was a time-dependent volume that applied constant pressure and temperature boundary conditions. Component 502 was a time-dependent junction that forced flow into the single-volume at a constant rate. The pressure and temperature in the model were set at the lowest values that still remained in the box of interest for the original steam tables (i.e. the lower left corner of the box). The flow rate was adjusted so that either the pressure or temperature reached the maximum value for the box at 10 s, at which time the calculation was terminated. Thus, the pressure and temperature of the single volume remained in the original box throughout the calculation. The measures for code performance were the normalized mass error and the rates of pressure and temperature increase. The analysis concentrated on the worst boxes in the various regions of the original thermodynamic grid. Calculations were performed with both the original and revised steam tables.

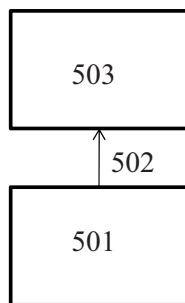


Figure 14. RELAP5-3D model used in the fill calculations.

The results of this analysis are summarized in Table 3. The table shows the box number, the pressure and temperature at the midpoint of the box, and the normalized mass error with the original and revised steam tables. For this evaluation, the normalized mass error was calculated as the absolute value of the mass error divided by the injected mass. Table 3 shows that the normalized mass errors were significant for the worst boxes in Regions 1 through 4 with the original steam tables. For example, the normalized mass error was greater than 40% for the worst box in Region 2. The table also shows that the normalized mass errors in these regions were reduced by more than an order of magnitude when the revised steam tables were used.

Table 3. Normalized mass errors during simple filling calculations.

Box	Midpoint values		Normalized mass error		Comments
	Pressure (MPa)	Temp. (K)	Original steam tables	Revised steam tables	
7556	17.25	622.5	1.08E-01	7.83E-03	Liquid (worst box in Region 1)
7669	18.25	627.5	6.18E-02	4.69E-03	Liquid (worst box in Region 3)
113	1.10E-03	275.33	7.67E-06	7.67E-06	Liquid (worst box in Region 7) <sup>1</sup>
7400	16.00	293.75	8.47E-06	5.30E-06	Liquid (worst box in Region 9) <sup>1</sup>
5629	7.50	377.5	7.24E-05	7.41E-05	Liquid (average box in Region 1)
7445	16.00	627.50	4.28E-01	5.63E-03	Vapor (worst box in Region 2)
7446	16.00	632.50	2.73E-01	1.02E-02	Vapor (worst box in Region 4)
341	1.50E-03	286.25	4.84E-04	4.84E-04	Vapor (worst box in Region 8)
1936	9.00E-02	410.0	4.67E-04	4.67E-04	Vapor (worst box in Region 10)
7495	16.00	936.575	3.88E-02	5.18E-03	Vapor (high temperature)
5651	7.50	617.50	3.33E-02	3.76E-03	Vapor (average box in Region 2)

<sup>1</sup>Worst box based on normalized error in specific volume rather than the coefficient of thermal expansion.

Table 3 shows that the normalized mass errors in Regions 7 through 10 were relatively small with the original steam tables. Because the normalized errors in the thermodynamic properties were generally small in Regions 1 and 2, the mass error with the original steam tables is also expected to be small for most of Regions 1 and 2. This expectation is confirmed by Boxes 5629 and 5651 that are representative of average, rather than maximum, errors in the coefficient of thermal expansion in Regions 1 and 2. The normalized mass error is very small for the liquid case, and although larger for the vapor case, is still acceptable from an engineering perspective.

The relatively large errors in the thermodynamic properties in portions of the thermodynamic grid have the potential to adversely affect parameters other than the mass error. Figure 15 shows the effects of the revisions to the steam tables on the pressure response during the fill problem for the worst vapor box in Region 2. The pressure was significantly affected by the changes to the steam tables. The average pressurization rate was about 14% higher with the revised steam tables. The pressure response was much more linear with the revised steam tables. Since the thermodynamic properties were more accurate with the revised steam tables and the mass error was much smaller, the pressure response was also probably more accurate with the revised tables. The results shown in Figure 15 suggest that the use of the original steam tables might cause the code to underestimate peak pressures during high-pressure operational transients that cause flow into the pressurizer.

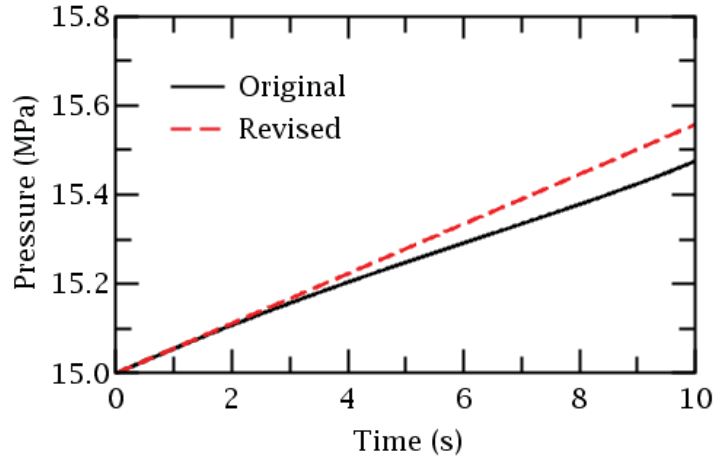


Figure 15. Calculated pressure during the fill problem for Box 7445.

A final fill problem was performed based on Box 7446, which was the worst box in Region 4. The calculation was identical to that described in Table 3 except that a higher fill rate was applied and the thermodynamic path inside Component 503 was allowed to extend beyond the original boundaries of Box 7446. The coefficient of thermal expansion for the vapor exhibited several minima and maxima during the calculation with the original steam tables as shown in Figure 16. These artificial minima and maxima were caused by a combination of the cubic interpolations used for the coefficient of thermal expansion in Subroutine sth2x6 and too coarse of a thermodynamic grid. The minimum values occurred at interior points in a box while the maximum values were associated with crossing the boundary of a box. The artificial minima and maxima disappeared when the revised steam tables were used because of their finer thermodynamic grid in this portion of Region 4.

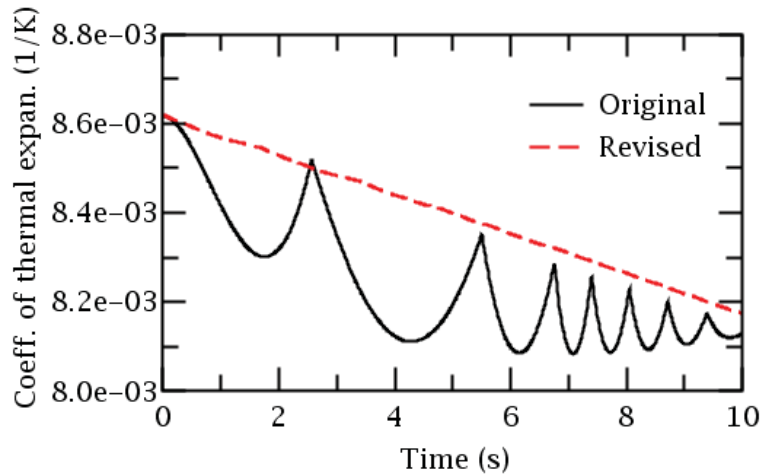


Figure 16. Vapor coefficient of thermal expansion during the fill problem for Box 7446.

The normal installation problems contained in the 'run', 'run/Athena', and 'run/Other' directories were calculated with the revised steam tables and compared to the results obtained with the original steam tables. Differences were observed for 23 of the installation problems. The effects of the steam tables on the mass error and CPU time at the end of the calculation were determined.

The effects were generally small on both mass error and CPU time. There were no clear trends with respect to mass error or CPU time. For example, the use of the revised steam tables caused the mass error to decrease in 12 of the installation problems, increase in 10, and remain constant in 1. The use of the revised steam tables caused the CPU time to decrease in 7 of the installation problems, increase in 14, and remain constant in 2.

A slightly modified version of one of the installation problem was used to look at the effects of the revisions to the steam tables more closely. This problem simulated a loss-of-coolant accident (LOCA) initiated by a small break in a PWR and was based on the installation problem typ12002.i. The working fluid was changed from h2on to h2o and the maximum time step size was varied between 0.1 and 0.01 s. The effects of the revisions to the steam tables and the time step size on the mass error are shown in Figure 17. With the larger time step size, similar results were obtained with the original and revised steam tables until about 850 s when the results diverged because of different loop seal clearing behavior. Experience with this model has shown a significant sensitivity concerning loop seal clearing. Typically one loop seal will clear, while the other loop seal remains plugged with liquid. The second loop seal will then clear and the first one will plug. The number of times that a loop seal might clear and plug can vary with different code versions. The differences shown in Figure 17 with the larger time step are similar to those observed previously between different code versions. The sensitivity of the calculated results to the steam tables decreased significantly when the maximum time step was reduced to 0.01 s.

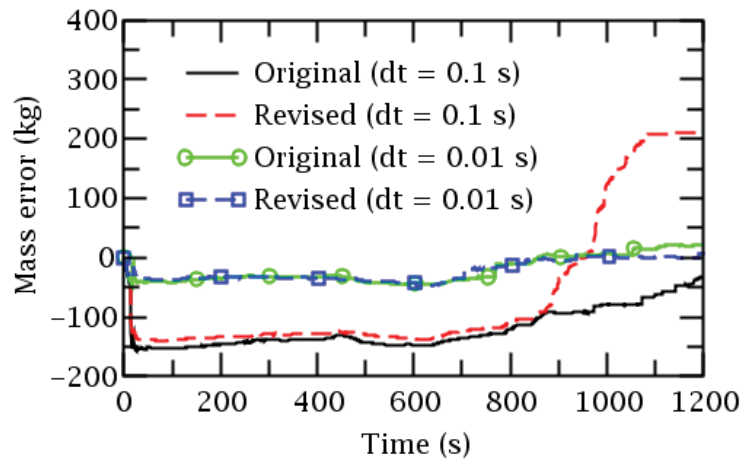


Figure 17. Mass error in the small-break LOCA calculations.

The CPU time required for the small-break LOCA calculations was not sensitive to the size of the steam tables. The use of the revised steam tables caused the CPU time to decrease by 0.7% with the larger time step, but to increase by 1.0% with the smaller time step.

## 6.0 Conclusions

The normalized errors in the interpolated thermodynamic properties at the midpoint of boxes for the original steam tables are documented in Section 5. These results indicate that the original thermodynamic grid is sufficiently detailed to provide acceptably accurate interpolations for most of Regions 1 and 2, which encompass the liquid and vapor regions required for most analyses of nuclear reactors cooled by light water. However, the evaluation also indicates that there are portions of Regions 1 and 2 where the original thermodynamic grid is not adequate. The largest errors occur in the vapor near the saturation line and are particularly large just above the normal PWR operating pressure of 15 MPa. The maximum normalized errors in specific volume and the



coefficient of thermal expansion are 0.024 and 0.217, respectively. Errors of this magnitude can cause excessive mass error and can adversely affect calculated pressurization rates during fill problems. The original steam tables were also judged to be inadequate for vapor temperatures between 800 and 1073.15 K.

The original steam tables were judged to be adequate at the low-pressure and/or low-temperature conditions needed for analysis of the balance of plant, which includes Regions 7 through 10 in this analysis.

Revised steam tables were created that used a finer temperature mesh between 530 and 640 K and between 800 and 1073.15 K and a generally finer pressure mesh between 4.0 and 21.5 MPa. The revised steam tables significantly reduced the relatively large errors that were observed in Regions 1 and 2 with the original steam tables. Large improvements were seen in the fill calculations for the worst boxes from the original grid. However, the more detailed steam tables did not provide a consistent reduction in mass error for the installation problems. In about half of the problems, including one based on a small-break LOCA in a PWR, the mass error actually increased with the more detailed steam tables. The conclusion from these calculations is that the more detailed steam tables will provide significantly improved results for a few cases, but will probably not have a large impact on most problems. The revisions to the steam tables do not significantly affect the CPU time required to run a problem.

The use of the original steam tables can result in relatively large property errors near the critical point and near the pseudo-critical line in the supercritical region. These regions were judged to be relatively un-important for analyses of most nuclear reactors cooled by light water. Therefore, the thermodynamic grid was not revised in these regions. A finer thermodynamic grid and/or improved interpolating algorithms are necessary to obtain better accuracy in these regions.

## 7.0 References

Haar, L, J. S. Gallagher, and G. S. Kell, *NBS/NRC Steam Tables: Thermodynamic and Transport Properties and Computer Programs for Vapor and Liquid States of Water in SI Units*, New York: Hemisphere, 1984.

Harvey, A. H., A. P. Peskin, and S. A. Klein, *NIST/ASME Steam Properties*, Version 2.2, Users' Guide, National Institute of Standards and Technology, U. S. Department of Commerce, NIST Standard Reference Database 10, March 2000.

MacDonald, P., J. Buongiorno, J. W. Sterbentz, C. Davis, and R. Witt, "Feasibility Study of Supercritical Light Water Cooled Reactors for Electric Power Production," INEEL/EXT-04-02530, Final Report, 12<sup>th</sup> Quarterly Report, January 2005.

Meyer, C. A., R. B. McClintock, G. J. Silvestri, and R. C. Spencer, Jr., *1967 ASME Steam Tables--Thermodynamic and Transport Properties of Steam Comprising Tables and Charts for Steam and Water*, New York, The American Society of Mechanical Engineers, 1967.

Nuclear Regulatory Commission, *NRC Regulations Title 10, Code of Federal Regulations, Part 50—Domestic Licensing of Production and Utilization Facilities, Appendix K to Part 50—ECCS Evaluation Models*, April 2010.

The RELAP5-3D Code Development Team, "RELAP5-3D Code Manual Volume I: Code Structure, System Models and Solution Methods," INEEL-EXT-98-00834, Revision 3.0, September 2009.